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Research article

Study of jack bean urease interaction with luteolin by the extended solvation model and docking simulation

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Abstract: In this study, the interaction between Luteolin and urease was made at 300 K in aqueous buffer solutions using isothermal titration calorimetry. The extended solvation model was used to calculate the solvation parameters. Moreover, to determine the interaction of Luteolin with Jack Bean Urease (JBU), a molecular docking process was performed. The purpose of this investigation was to measure the inhibitory effects of Luteolin on the activity and structure of urease. Molecular docking analysis confirmed the extended solvation model.

Keywords: Isothermal Titration Calorimetry; luteolin; the extended solvation theory; inhibitor; docking

1. Introduction

The question of finding effective and useful inhibitors of urease enzyme has been in the interest of researchers for many years. JBU is a urea amidohydrolase, this metalloenzyme contains two nickel ions per subunit and is widely found in soil, plants, and microscopic organisms like bacteria, algae, fungi, and invertebrates [1].

Urease is responsible for the hydrolysis of urea to carbon dioxide and ammonia. The mechanism of urea hydrolysis is widely proposed by many researchers .The metal cations interact with hydroxyl ions, and the three molecules of water immerse in the active site of the enzyme [1]. Since urea contains two hydrogen bonding sites, one carbonyl group, and the other amino acid group, hydrogen bond formation plays an important role in the binding of urea to the two nickel atoms